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Shallow-donor states in spherical quantum dots with parabolic confinement

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ABSTRACT

The evidence of a parabolic potential well in quantum wires and dots was reported in the literature, and a parabolic potential is often considered to be a good representation of the "barrier" potential in semiconductor quantum dots. In the present work, the variational and fractional-dimensional space approaches are used in a thorough study of the binding energy of on-center shallow donors in spherical GaAs-$Ga_{1-x}Al_xAs$ quantum dots with potential barriers taken either as rectangular [$V_b(\text{eV}) = 1.247\ x$ for $r > R$] or parabolic [$V_b(r) = \beta^2 r^2$] isotropic barriers. We define the parabolic potential with a β parameter chosen so that it results in the same E_0 ground-state energy as for the spherical quantum dot of radius R and rectangular potential in the absence of the impurity. Calculations using either the variational or fractional-dimensional approaches both for rectangular and parabolic potential result in essentially the same on-center binding energies provided the dot radius is not too small. This indicates that both potentials are alike representations of the quantum-dot barrier potential for a radius R quantum dot provided the parabolic potential is defined with β chosen as mentioned above.

INTRODUCTION

Quantum-dot heterostructures are most studied both from the theoretical and experimental point of view due to the wide possibility of applications in electronic and optoelectronic devices [1]. Such semiconductor nanostructures show interesting physical properties due to the extreme degree of confinement of electrons and holes, and the presence of impurities of course modify both the optical and transport properties of such nanostructures. For impurities in quantum dots, the ultimate goal is an artificial atom whose properties can be controlled through the material parameters and geometry.

Using variational and fractional-dimensional space approaches, Porras-Montenegro and Pérez-Merchancano [2] and Oliveira et al. [3] have calculated the binding energy for shallow-donor impurities in rectangular GaAs-(Ga,Al)As quantum dots for both finite and infinite potential confinement. As a general feature, they have found that the binding energy increases as the radius of the dot is diminished and then decreases to the three dimensional limit of the bulk in the case of finite potential confinement, whereas the binding energy always increases with the diminishing of the radius of the dot when the potential confinement is infinite.

The evidence of a parabolic potential well in quantum wires and dots was reported in the literature [4, 5], and a parabolic potential is often considered to be a good representation of the "barrier" potential in semiconductor quantum dots [6-8]. The theoretical description of the behavior of a hydrogenic on-center donor in a spherical dot for rectangular and parabolic potentials will lead to a better understanding of the properties of a spherical quantum dot, and it is

the subject of this paper. Calculations have been made within the effective mass approximation and using a variational and the fractional-dimensional space approaches.

THEORETICAL FRAMEWORK

Within the effective-mass approximation, the Hamiltonian of a system consisting of an electron bound to a donor impurity, inside a GaAs-(Ga,Al)As quantum dot of radius R for a parabolic potential confinement, may be written as

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{1}{2}m^*\omega^2 r^2 - \frac{e^2}{\varepsilon_0 r}\ , \qquad (1)$$

where r is the electron-impurity distance, ε_0 (= 12.58) is the dielectric constant of bulk GaAs, m^* (= 0.0665 m_0, where m_0 is the free electron-mass) is the effective electron mass, and ω is the harmonic oscillator frequency.

In the variational calculation, the trial wave function for the ground state with the impurity present is taken [8] as the product between the eigenfunction of the Hamiltonian in eq. (1) without the Coulomb interaction (third term at the right) and the hydrogenic part, i.e.:

$$\psi(r) = N \exp(-\beta r^2/2) \exp(-\lambda r)\,, \qquad (2)$$

where N is a normalization constant, λ is a variational parameter, and β is a measure of the parabolic potential, defined as

$$\beta = \frac{m^*\omega}{\hbar}\ . \qquad (3)$$

Alternatively, one may solve the above problem in the fractional-dimensional scheme. Following Oliveira et al. [3], one finds that, for the 1s-like ground state, the "shallow donor + heterostructure" anisotropic system may be modeled by an effective isotropic hydrogenic system in a fractional D-dimensional space, a problem which may be solved analytically. Once the fractional dimension is calculated, the donor binding energies may be obtained [9, 10] through $E_b = -E_{1s} = 4R^*/(D-1)^2$, where R^* is the donor effective Rydberg. For details of calculations we refer to [3].

RESULTS AND DISCUSSION

In Figure 1 (a) we present the spherical parabolic and rectangular potential profiles for an R = 200 Å GaAs-$Ga_{1-x}Al_xAs$ quantum dot with an Al concentration x = 0.3; we have chosen β and R so that both potentials result in the same E_0 ground-state energy. In Figure 1 (b) it is displayed the parabolic-potential parameter $\beta^{-1/2}$ versus dot radius R.

Figure 2 displays the on-center donor binding energy versus quantum dot radius for a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum dot calculated both for a parabolic (dotted line) and rectangular (full curve) potentials. Calculations are performed using a variational procedure [cf. Fig. 2 (a)] and the fractional-dimensional approach [Fig. 2 (b)]. In both cases one observes that the binding energy diminishes with increasing radius of the dot, reaching the three–dimensional limit (the hydrogenic atom) for large values of the radius, as it is has been reported in several works [2, 3]. As it can be seen, the agreement in the binding energy between the variational method and the fractional-dimensional approach is quite good in a wide range of the radius of the dot, independently whether the confinement is parabolic or rectangular. For radius smaller than $\approx$ 2 - 3 a^* the binding energy calculated by means of the two methods begins to differ, and the fractional-dimensional approach begins to fail [3].

CONCLUSIONS

Summing up, using the variational and fractional-dimensional approaches both for rectangular and parabolic potentials we have calculated the binding energy of an on-center donor impurity in a GaAs-(Ga,Al)As quantum dot. We find the results essentially the same provided the dot radius is not too small. This indicates that both potentials are alike representations of the quantum-dot barrier potential for a radius R quantum dot provided the parabolic potential is defined with β as it was chosen in this work. We do hope that this criteria may be of future utility in calculations

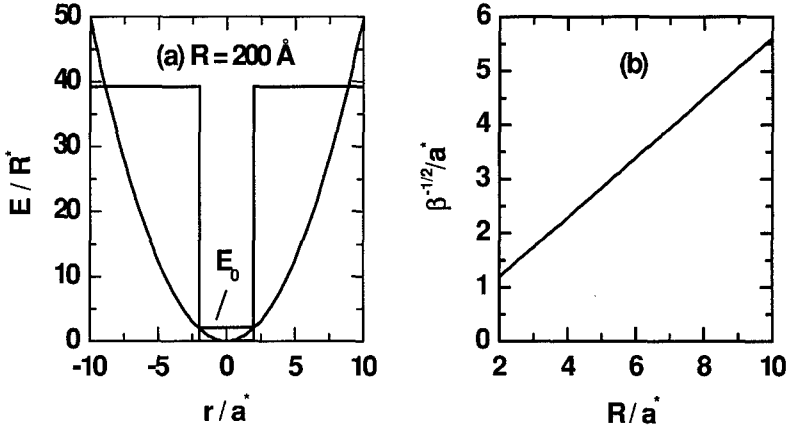

Figure 1: (a) spherical parabolic [$V_b(r) = \beta^2 r^2$] and rectangular [$V_b(\text{eV}) = 1.247\ x$ for $r > R$] potential profiles for an R = 200 Å GaAs-$Ga_{1-x}Al_xAs$ quantum dot ($x = 0.3$); β and R are chosen so that both potentials result in the same E_0 ground-state energy; (b) parabolic-potential parameter $\beta^{-1/2}$ versus dot radius R. In the above figures, R^* and a^* are the effective Rydberg and Bohr radius, respectively.

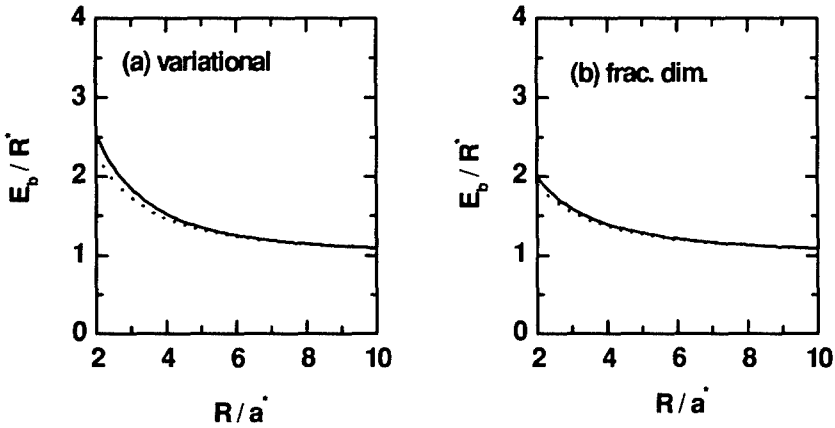

Figure 2: On-center donor binding versus quantum dot radius for a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum dot calculated both for a parabolic (dotted line) and rectangular (full curve) potentials. Calculations are performed using a variational procedure (a) and the fractional-dimensional approach (b).

using the parabolic potential for impurity-related properties in low-dimensional systems, such as impurity binding and transition energies, as well as theoretical work on photoluminescence and absorption spectra.

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